1,3-Naphthalenediol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.06

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found
1,5-Dihydroxynaphthalene
Measured: 1.94
Predicted: 1.59

Image not found
1,3-Naphthalenediol
Measured: 1.97
Predicted: 2.06

Image not found
1,4-Naphthalenediol
Measured: 1.90
Predicted: 1.93

Image not found
Benzenebutanoic acid, .gamma.-oxo-
Measured: 1.30
Predicted: 1.43

Image not found
Benzoic acid, 5-bromo-2-hydroxy-
Measured: 3.23
Predicted: 2.50